netlog

NETL's R&D newsletter

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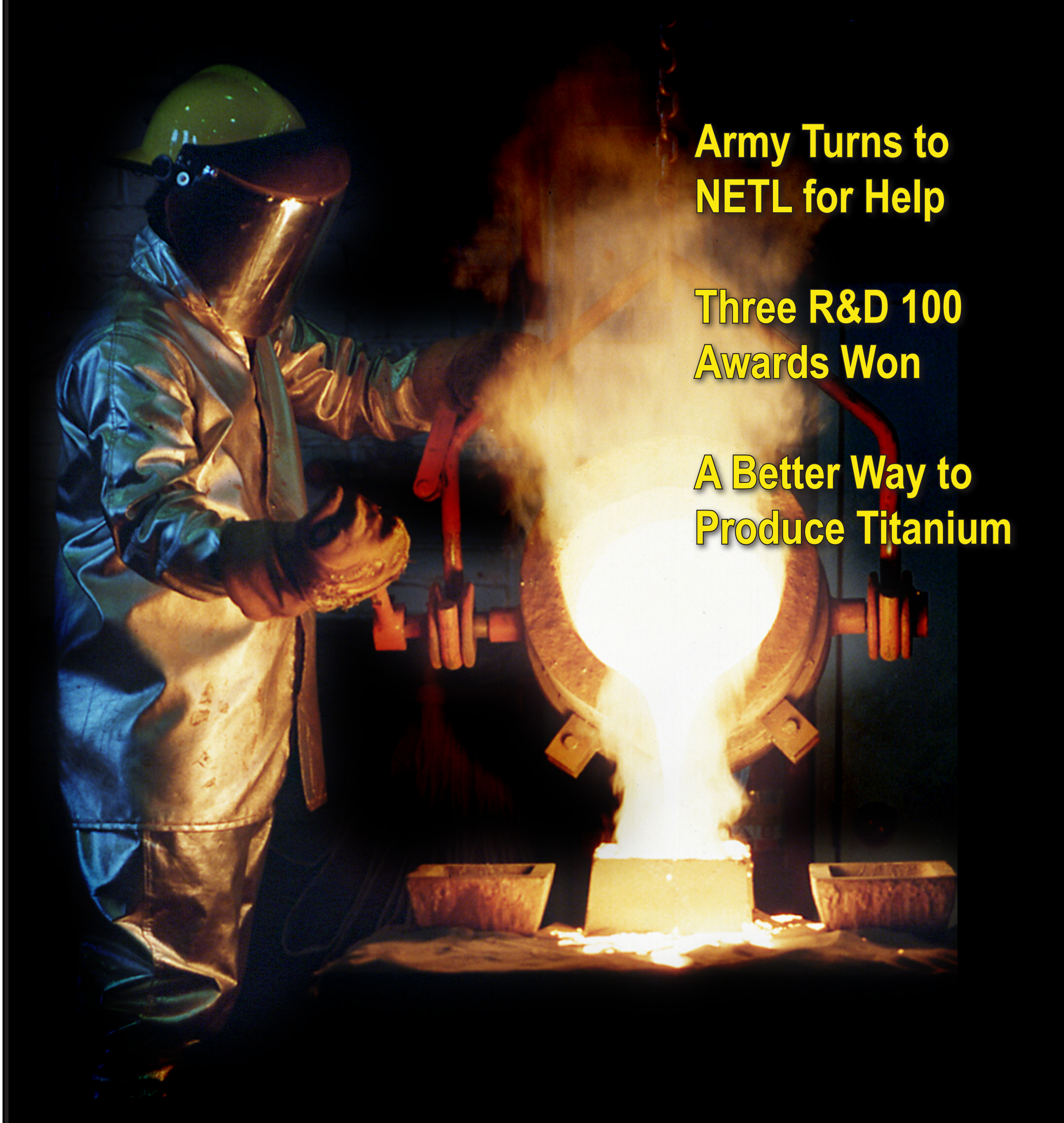

Army Turns to NETL for Help

Three R&D 100 Awards Won

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ON THE COVER

A technician at NETL pours molten steel into a P-900 mold during the process to create cast-steel armor plates for military vehicles.

netlog is a quarterly newletter which highlights recent achievements and ongoing in-house research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

U.S. Army Seeks NETL's Help to Commercialize Cast Steel Armor

The U.S. Army Tank and Automotive Command (TACOM) has asked for NETL's help in procuring 10 million pounds of P-900 cast steel armor to be used as an add-on to certain military vehicles to protect them from improvised explosive devices (IEDs).

NETL is the only source of production-sized patterns for the armor. NETL researchers are supplying technical expertise along with polystyrene P-900 patterns to foundries for use in making test targets.

The Army wants the first 2.5 million pounds of armor to be delivered during the last quarter of this calendar year.

Earlier this year, NETL scientists produced the original castings for the slotted steel armor using a new heat treatment to maximize protection against IEDs. Ballistic tests performed on the NETL-produced test plates proved so successful that the Army decided to issue a market call for production of armor.

NETL researchers are also reviewing the information supplied from the foundries to TACOM as a result of the market call. Each foundry producing the castings will have to be qualified for its ballistic and production-business plan. Many of the foundries plan to use the lost-foam casting method for steel pioneered by NETL scientists in the 1990s. NETL also volunteered its tooling to have additional patterns made to help jump-start the production process while others await full-size patterns. NETL personnel will visit some of the foundries and the Army Research Laboratory to help determine their qualifications.

The Army has a $3 million budget to help a number of foundries get the tooling and allow them to make enough prototype castings to get them qualified. The plan is then to go into full-scale production.

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Government, Industry Team Develops Better Way to Produce Titanium

NETL researchers Steve Gerdemann, Paul Jablonski, and Paul Turner have been working with International Titanium Powder, LLC (ITP) of Rockport, IL, for the past 9 years to refine ITP's method to reduce the cost of producing titanium and titanium alloys. The groundbreaking method, called the Armstrong Process, deviates from the "traditional" methods for titanium production in that it's a continuous process, rather than a batch-at-a-time, eliminating the down-time associated with a step-wise batch process. Continuous production allows for lower temperatures and lower pressure, which in turn means lower cost. Recently, the team has developed methods to economically turn Armstrong Process powders into usable, economical products for the automotive, defense, and aerospace industries using both single-melt and solid-state compaction technologies.

The prototype ingot made from Armstrong Process titanium is being removed from the preheat furnace for hot working.

This technology won a prestigious R&D 100 award this year.

What's so great about titanium? It's strong, it's lightweight, and it resists corrosion. In fact, titanium has the highest strength-to-weight ratio of any metal. It's strong as steel, but nearly half as dense. Although the metal was discovered in 1791, it was confined to laboratory use until the invention of the Kroll process in 1946 because extracting titanium from its ores is a long and expensive process. Even so, the high-temperature Kroll process (a batch process commercialized at NETL in the late 1940s) currently used for manufacturing titanium is so expensive that titanium can be practically used only in specific, high-priced markets. The new cost-efficient Armstrong process opens up titanium to a variety of applications. One noteworthy example is NETL's work with the U.S. Army Tank and Automotive Command and Army Research Laboratory in developing armor plate. Titanium armor plate possesses the light-weight, high-corrosion resistance properties of titanium.

ITP has broken ground on its first commercial plant, which should be operational by the first quarter of 2009. A significant portion of that plant's production is already committed under multi-year, extended contracts. Department of Defense contractors are planning to use this product in their defense-related products. The Armstrong Process and applications for its products were developed by a team composed of International Titanium Powder, LLC (Rockport, IL), NETL, Oak Ridge National Laboratory (Oak Ridge, TN), BAE Systems (Rockville, MD), AMETEK (Paoli, PA), and Red Devil Brakes (Mount Pleasant, PA).

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NETL Wins Three 2007 R&D 100 Awards

Three technologies developed by researchers at NETL have been selected this year by an independent judging panel and the editors of *R&D Magazine* as among the 100 most technologically significant products introduced into the marketplace in 2007.

First, the latest release of NETL's Multiphase Flow with Interphase eXchanges (MFIX) software—developed for modeling multiphase reactors such as coal gasifiers encountered in fossil fuel processing plants—bests competing computational fluid dynamics products by its phenomenological fidelity in describing heavily loaded gas-solids flows in both continuous and discrete terms, and its use of an open-source methodology to disseminate information and receive developmental feedback. Second, SEQURE™ well-finding technology, developed in partnership with Apogee Scientific, Inc. (Englewood, CO), Fugro Airborne Surveys (Mississauga, Ontario), and LaSen, Inc. (Las Cruces, NM), will aid significantly in geological carbon sequestration by rapidly, accurately, and cost-effectively locating wells—even if unknown or mislocated—that could represent leak sources. Third, the Armstrong Process CP Ti and Ti Alloy Powder and Products along with NETL, Oak Ridge National Laboratory, and four private companies developed a breakthrough method for producing titanium powder continuously and at lower cost, representing the most significant development in the titanium industry in 50 years.

Recognized by industry, government, and academia, an R&D 100 Award provides an important boost to new products just entering the marketplace. All of this year's R&D 100 awards are displayed in the September issue of *R&D Magazine*.

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Neetha Khan, a research scientist at NETL, prepares an experiment with iron nanoparticles in NETL's Omicron Analysis and Surface Imaging System. Research Group Leader Brad Bockrath, standing left, and Project Leader Chris Matranga observe the generation and analysis of the nanoparticles.

Fundamental Studies Conducted on Iron-Based Model Catalysts

NETL researchers are using one of their newest and most powerful scientific instruments to learn important information about iron nanoparticles. The researchers have generated and analyzed novel nanoscale iron particles in the first experiments using the Omicron Analysis and Surface Imaging System (OASIS), a state-of-the-art ultra-high-vacuum surface-science instrument. The successful synthesis of these particles is a first step toward being able to study the adsorption properties of these nanoparticles. Studies on nanostructured materials such as these iron oxide nanoparticles can help researchers understand the importance of specific adsorption sites, such as the particle edges that play a critical role in catalysis.

Iron is the basis for many catalysts, such as those used in the Fischer-Tropsch synthesis of transportation fuels. To gain a better understanding of materials used in Fisher-Tropsch applications, this new work focuses on fundamental studies of the fabrication of iron and iron oxide on gold surfaces that serve as model nanocatalysts.

The particles were synthesized in situ and analyzed using surface-sensitive techniques that provide information about particle composition and structure.

The OASIS instrument allows researchers to image individual atoms and determine the elemental composition of the first few atomic layers of surfaces relevant to fossil energy applications. The system incorporates such analytical and atomic imaging systems as X-ray photoelectron spectroscopy, Auger electron spectroscopy, ion scattering spectroscopy, low-energy electron diffraction, electron energy loss spectroscopy, scanning tunneling microscopy, and atomic force microscopy into one single ultra-high-vacuum system.

Contact:
Bradley Bockrath, 412-386-6081

Novel Low-Swirl Fuel Injector (LSI) Shows Potential for Combustion of High Hydrogen Fuels

Results of tests conducted in the NETL High-Pressure Combustion Facility, which allows for direct observation and imaging of combustion flames at elevated pressure, show that the LSI has potential for stable, low-emission operation with high-hydrogen fuels. Stable operation was achieved at pressures ranging from 1 to 8 atmospheres, over a range of nozzle velocities (20 – 60 m/s), with fuel-gas mixtures approaching 100 percent hydrogen. Developed and patented at Lawrence Berkeley National Laboratory, LSI is a simple, robust, very cost-effective technology that can increase system efficiency while maintaining ultra-low emissions of NO_x and carbon monoxide. NETL researchers have collaborated in evaluating LSI potential for achieving FutureGen emissions goals under the Fossil Energy Turbine Technology R&D Program.

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Thomas Simonyi, left, and Stephen Beer use a thermogravimetric analyzer to analyze heavy metals to determine their suitability for making thin-film sensors for natural gas.

New Technique Developed to Assess Catalyst Activity with Fuel Gases

Researchers in the Energy System Dynamics Division of NETL's Office of Research and Development are teaming with Carnegie Mellon University and West Virginia University to develop sensor arrays that can respond to rapid changes in fuel-gas composition.

The ability to detect and respond to changes is increasingly important because of the anticipated increased usage of liquefied natural gas in the nation's pipeline system. This University Research Initiative project will take advantage of an analytical technique developed by NETL researchers.

The technique for sensing hydrocarbons such as methane (C1), ethane (C2) and propane (C3) involves characterizing their cracking behavior over catalyst materials. This technique differentiates the activity of platinum metal catalysts with C1-C3 gases from thermal cracking.

The results indicate this method should increase the sensitivity of future tests to changes in parameters, including pressure, catalyst particle size, and gas flow rates.

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Tests Identify Potential Additive for Synthetic Jet Fuel

Based on experimental results involving two important synthetic jet fuel performance parameters, benzyl alcohol was identified as the best candidate from a series of potential compounds to be used as an additive to promote seal swelling. Additional testing of the fuel to measure its performance relative to other fuel specification properties must still be conducted before the additive can be recommended. Synthetic jet fuel produced from coal-derived synthesis gas has the potential for lessening the military's dependence on foreign sources of petroleum.

The highly paraffinic nature of the fuel can result in insufficient seal swelling of elastomer components of jet fuel systems, leading to fuel leaks. Thermal stability tests of mixtures of benzyl alcohol and a surrogate jet fuel showed that it does not degrade thermal stability of the fuel. ASTM swelling tests showed that an acceptable level of nitrile rubber seal swelling can be achieved with concentrations as low as 0.5% by volume of benzyl alcohol.

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New NETL Material Exhibits Unusual Gas Adsorption Behavior

Researchers have engineered an absorbent material with an unusually flexible structure that offers exciting possibilities for gas separation, gas purification, and gas sensing devices. The material is composed of sheets of an iron-nickel complex inter-layered with pillars of a specially selected organic compound to form galleries of open channels into which gas molecules can fit. In the presence of carbon dioxide at a certain threshold pressure, the structure flexes opens to accommodate more gas molecules. Once full, the opened structure retains carbon dioxide despite depressurization until a very low pressure is reached, whereupon the structure collapses again as the carbon dioxide exits. Achieving such a degree of control over the properties of a family of porous materials represents a real advance in adsorption science.

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Video Feature

NETL, University Report Results of Interaction of Toxic Industrial Compounds with Alumina Surface

In a recent collaborative effort, NETL computation-chemistry scientist Dan Sorescu and scientists at the University of Pittsburgh reported their results related to the interaction of toxic industrial compounds with hydrogen cyanide (HCN). The link of atomistic evidence obtained with sophisticated surface science capabilities to computational chemistry modeling performed at NETL research facilities proved one more time a successful approach to generate scientific insight. The study was published in the *Journal of Physical Chemistry*.

This study showed that, in addition to molecular bonding, aluminum ion sites act as centers of dissociation for HCN molecules. It further demonstrates that accuracy of computational models based on first-principle calculations is very similar to the data obtained using highly accurate spectroscopic techniques. The results obtained in this work can be further extended to other types of toxic industrial compounds such as cyanogen chloride (ClCN), sulfur dioxide (SO_2), or hydrogen sulfide (H_2S) where the role played by various amine-decorated oxide surfaces in facilitating molecular adsorption can be tested in detail.

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Evan Granite in front of the packed bed reactor, which he uses to conduct research into capturing mercury, arsenic, and selenium. Granite's patented capture technologies have been licensed to industry for use in the electric power generation industry.

Researchers Publish Paper on Impact of Sulfur Trioxide on Mercury Capture

A paper by NETL researchers on how sulfur oxides impact mercury capture by activated carbon was published in the American Chemical Society journal *Environmental Science & Technology*.

Recent field tests of mercury removal with activated carbon injection (ACI) have revealed that mercury capture is limited in flue gases containing high concentrations of sulfur oxides (SO_x).

To gain a better understanding of the impact of SO_x on ACI, mercury capture was tested under varying conditions of SO_2 and SO_3 concentrations using a packed-bed reactor and simulated flue gas (SFG). The final mercury concentration of the activated carbons is independent of the SO_2 concentration in the SFG, but the presence of SO_3 inhibits mercury capture even at the lowest concentration tested (20 parts per million). The mercury removal capacity decreases as the sulfur content of the used activated carbons increases from 1 to 10 percent. In one extreme case, an activated carbon with 10 percent sulfur, prepared by sulfuric acid impregnation, shows almost no mercury capacity. The results suggest that mercury and sulfur oxides are in competition for the same binding sites on the carbon surface. The poisoning of activated carbon by sulfur trioxide is a difficult issue to resolve. Sulfur trioxide is often injected upstream of an electrostatic precipitator to enhance capture of particulates. During combustion of high-sulfur coals, as much as 1-2 percent of the sulfur is converted to sulfur trioxide, leading to flue gas concentrations in the range of 10-40 parts per million. Sulfur trioxide also forms by oxidation of sulfur dioxide across an SCR catalyst. Possible solutions include co-injection of alkaline sorbents with the activated carbon, flue gas desulfurization upstream of the ACI, and the use of alternative fly ash conditioning agents. Each of these potential solutions comes with significant drawbacks, including additional cost for the utility operators.

Contact:
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Researchers Invent Mercury Detection Technology

NETL inventors Evan Granite and Henry Pennline have added a mercury detection technology to their portfolio of mercury removal technologies. Previously they patented three mercury control technologies that have been licensed to industry for commercial use in removing mercury from coal-derived flue gases. Their new invention detects mercury in flue gases, which will make it possible for power plants to verify that they are complying with regulations either issued or pending at the Federal level and in 26 states. The detection technology can be used with any mercury removal technology to determine how much mercury is present before the coal is burned and how much remains after combustion. NETL has applied for a patent. The technology is a spinoff of the GP-254 removal technique which irradiates flue gas with ultraviolet light.

The new technique works by blending a small slipstream of hot flue gas with oxygen or air, and subsequently irradiating it with 254-nanometer ultraviolet light. This results in quantitative deposition of the mercury as mercuric oxide, allowing for the rapid determination of concentration in flue gas. The United States Environmental Protection Agency recently issued a regulation for the reduction of mercury emissions from coal-burning utilities. Twenty six states have legislation or pending legislation for mercury control on coal-fired power plants. Mercury is present within coal-derived flue gases at infinitesimally small concentrations. The typical concentration of mercury in untreated coal-derived flue gas is on the order of one part-per-billion, while treated flue gases often have sub part-per-billion mercury levels.

Contact:
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Sheila Hedges, a research chemist at NETL, examines a fine precipitate forming in a groundwater sample after an experiment conducted to examine chemical changes during carbon dioxide storage in unmineable coal seams.

NETL Researchers Study CO_2 Sequestration in Unmineable Coal Seams

Researchers in the Geosciences Division of NETL's Office of Research and Development have shown that changes to the produced water chemistry and the potential for mobilizing toxic trace elements from coalbeds are important factors to be considered when evaluating deep, unmineable coal seams for CO_2 sequestration.

A team of researchers, led by Dr. Sheila Hedges, conducted an initial investigation into the potential environmental impacts of CO_2 sequestration in unmineable coal seams.

The research focused on changes in the produced water during enhanced coalbed methane production, using a CO_2 injection process. Details of this exploratory evaluation of mobilization of trace elements from coal have been published in the most recent issue of *International Journal of Environment and Pollution*.

A high-volatile bituminous coal, Pittsburgh No. 8, was reacted with synthetic produced water and gaseous carbon dioxide to evaluate the potential for mobilization of toxic metals during CO_2-enhanced coalbed methane sequestration.

Microscopic and X-ray diffraction analysis of the post-reaction coal samples clearly show evidence of chemical reaction, and chemical analysis of the synthetic produced water shows substantial changes in composition.

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Robert McLendon adjusts the CT scanner used during research at NETL. The scanner is used mainly to measure in-situ fluid displacement and sorption of fluids within mineral cores

NETL Researchers Use CT Scan To Study Carbon Dioxide in Coal

When most people think of a CT scan, the image that comes to mind is lying on a narrow support, being told not to move, and being inside a round opening where mysterious technology produces X-ray images of relevant parts of their bodies.

But NETL researchers in the Office of Research and Development are using the same computerized X-ray tomography (CT) to measure carbon dioxide concentrations throughout coal cores. This type of research is essential as policy-makers decide whether or not they will try to deal with excess carbon dioxide by storing it permanently in geologic formations.

NETL researchers have been studying apparent sorption in coal cores under confining pressure. A paper describing NETL experiments on carbon dioxide transport and sorption behavior in confined coal cores for enhanced coalbed methane and carbon dioxide sequestration has been accepted for inclusion in the proceedings of the Society of Professional Engineers (SPE) National Meeting, Anaheim, CA, Nov. 11-14.

Measurements of sorption isotherms and transport properties of CO_2 in coal cores are important for designing enhanced coalbed methane/CO_2 sequestration field projects. Sorption isotherms measured in the lab can provide the upper limit on the amount of CO_2 that might be sorbed in these projects.

The isotherms are commonly measured for samples of powdered coal; use of a powder, while convenient, prohibits the application of a mechanical confining pressure to the sample. Because sequestration will most likely occur in unmineable coals, those coals will be under considerable pressures. Measurements on powdered coal cannot account for the lithostatic pressures present in coal seams.

The study of Pittsburgh No. 8 coal, an important bituminous coal, showed that gas sorption advanced at different rates in different regions of the core and that diffusion and sorption progressed slowly. The amounts of CO_2 sorbed were plotted vs. position (at fixed times) and vs. time (for various locations in the sample). The resulting sorption isotherms were compared to isotherms obtained for powdered coal from the same Pittsburgh No. 8 sample. The results show that for this coal, the apparent sorption isotherms were dependent on position of the volume element in the core and the distance from the CO_2 source. Also, the calculated isotherms show that the coal core sorbed somewhat less CO_2 than the powdered coal. Changes in density distributions during the experiment were also observed. After desorption, the density distribution of calculated volume-elements differed from the initial distribution, suggesting a rearrangement of coal structure due to CO_2 sorption.

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NETL, RMOTC, and Fugro Airborne Surveys collaboration uses a helicopter and aeromagnetics to make a comprehensive inventory of wells, pipelines, and other oilfield infrastructure. Sensors on board will measure methane emissions from various sources including wellheads, pipelines, production facilities, and produced-water ponds.

SEQURE™ Well-Finding Technology Used to Locate Wells and Methane Leaks

SEQURE™ well-finding technologies deploy sensitive magnetic and methane sensors on highly mobile platforms to locate abandoned and leaking wells on very large tracts of land, thereby saving time and money. NETL's SEQURE™ technology, which won this years R&D 100 award referred to earlier in this issue, was used to survey the Naval Petroleum Reserve No. 3 (NPR-3), a 15-square-mile oilfield near Casper, WY. Over 1,500 line kilometers of magnetic and methane data were acquired from a helicopter using boom-mounted magnetometers and a sensitive methane and light hydrocarbon detector. NETL modified the flight plan and instrument payload used previously for the highly successful 2005 SEQURE™ well-finding survey at the nearby Salt Creek Oilfield to improve the detection of wells with weak magnetic signatures. In addition, the methane detection device was added to detect any leaking infrastructure in the 100-year-old oilfield.

To evaluate the effectiveness of the helicopter survey, NETL scientists conducted a thorough ground-level magnetic and methane survey of a 100-acre test area within the NPR-3 survey area for comparison. NETL will process the airborne data and provide the U.S. Strategic Petroleum Reserve with GIS maps depicting anomalous magnetic features and methane plumes as overlays. Initial maps using uncorrected magnetic data depict the location of numerous, weak, well-type anomalies, a preliminary indication that the survey was successful.

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